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Clustering of Natural and Nature Derived Compounds for Cardiovascular Disease: Pharmacophore Modeling

Authors : S. Roy, R. Rekha, K. Sriram, G. Subhadra, R. Johana

Abstract : Cardiovascular disease remains a leading cause of death in most industrialized countries. Many chemical drugs are available in the market which targets different receptor proteins related to cardiovascular diseases. Of late the traditional herbal drugs are safer when compared to chemical drugs because of its side effects. However, many herbal remedies used in treating cardiovascular diseases have not undergone scientific assessment to prove its pharmacological activities. There are many natural compounds, nature derived and Natural product mimic compounds are available which are in the market as approved drug. In the most of the cases drug activity at the molecular level are not known. Here we have categorized those compounds with our experimental compounds in different classes based on the structural similarity and physicochemical properties, using a tool, Chemmine and has attempted to understand the mechanism of the action of a experimental compound, which are clustered with Simvastatin, Lovastatin, Mevastatin and Pravastatin. Target protein molecule for Simvastatin, Lovastatin, Mevastatin and Pravastatin is HMG-CoA reductase, so we concluded that the experimental compound may be able to bind to the same target. Molecular docking and atomic interaction studies with simvastatin and our experimental compound were compared. A pharmacophore modeling was done based on the experimental compound and HMG-CoA reductase inhibitor.

Keywords : molecular docking, physicochemical properties, pharmacophore modeling structural similarity, pravastatin
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